The Institute for Shock Physics SEMINAR SERIES

Presents

Building a Computational Framework to Model Dynamic Behavior Materials

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The dynamic response of metallic materials involves a complex interplay between plasticity mechanisms and the spatial and temporal evolution of stress states and temperatures that determine how materials respond and fail. Recent advances allow the characterization of these mechanisms in real time using *in situ* diffraction experiments (XRD). However, the ability to quantify the contributions from these mechanisms is lacking using experiments alone.

This talk will highlight the capabilities of classical molecular dynamics (MD) simulations to unravel the contributions from dislocation slip, deformation twinning, and phase transformation in metallic materials under shock-loading conditions. In addition, the coupling of MD simulations with a two-temperature model (TTM) allows the modeling of laser-metal interactions to understand the role of ablation and melting on the dynamic behavior of materials. Atomic scale microstructures enable the use of simulated diffractograms at various stages of loading to understand the contributions of deformation mechanisms to peak shifts/splitting/broadening behavior and complement the interpretation of experimental results. A new virtual texture (VirTex) analysis tool is developed to generate simulated EBSD maps and characterize the microstructure signatures of the dynamic deformation and failure behavior as carried out experimentally using recovered samples. However, the computational costs associated with MD simulations limit their ability to complement the interpretation of experimental results. A new quasi-coarse-grained dynamics (QCGD) framework is developed that extends the capability of MD simulations to the experimental scales to model the dynamic behavior of materials and predict the microstructure evolution at the time/length scales of in situ experiments. The various computational methods and the ability to recreate the *in situ* shock experiments and serve as a digital twin framework will be presented.

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Shock Physics Building || Seminar Room 201

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